

NIST Chemistry WebBook

Version History

August 1996

- First release
- Contains data from NIST Standard Reference Database 19A: *NIST Positive Ion Energetics*, v. 2.0.
- Database contents (11,000+ total species):

Data Type	Number of Species
Thermochemical data and estimates	5,000+
Gas phase ion energetics data	10,000+

February 1997

- Neutral thermochemistry archive added.
- Condensed phase heat capacity archive added.
- Heat of sublimation database added.
- Boiling point and vapor pressure data added.
- IR and mass spectra added.
- Additional ionization energy and appearance energy data added.
- Proton affinity and gas basicity evaluations added.
- Estimated and uncertain thermodynamic data from NIST Standard Reference Database 19A removed.
- Database contents (22,300+ Total species):

Data Type	Number of Species
Gas phase thermochemical data	2,800+
Condensed phase thermodynamic data	4,600+
Phase change thermodynamic data	7,800+
Reaction thermodynamic data	4,500+
Gas phase ion energetics data	12,700+
IR spectrum	5,200+
Mass spectrum	8,300+

August 1997

- Fluid property data added.
- Negative ion energetics data added.
- Additional positive ion energetics data added.
- Additional data from the neutral thermochemistry archive added.
- Database contents (27,300+ Total species):

Data Type	Number of Species
Gas phase thermochemical data	2,800+
Condensed phase thermodynamic data	4,600+

Phase change thermodynamic data	8,800+
Reaction thermodynamic data	7,400+
Gas phase ion energetics data	14,200+
IR spectrum	5,200+
Mass spectrum	8,300+
Fluid property data	13

March 1998

- Vibrational and electronic energy levels for transient polyatomic molecules added.
- Constants of diatomic molecules added.
- Organometallic thermochemistry archive added.
- Updates provided for many of the datasets previously added to the site.
- Database contents (31,600+ Total species):

Data Type	Number of Species
Gas phase thermochemical data	5,800+
Condensed phase thermodynamic data	5,300+
Phase change thermodynamic data	9,400+
Reaction thermodynamic data	8,700+
Gas phase ion energetics data	14,300+
IR spectrum	5,200+
Mass spectrum	10,600+
Vibrational & electronic energy levels	2,600+
Constants of diatomic molecules	600+
Fluid property data	16

November 1998

- Additional vibrational energy levels added.
- Henry's law constant database added.
- UV/Vis spectra added.
- Additional critical property data added.
- Updates provided for many of the datasets previously added to the site.
- Database contents (31,600+ Total species):

Data Type	Number of Species
Gas phase thermochemical data	6,100+
Condensed phase thermodynamic data	5,500+
Phase change thermodynamic data	9,500+
Reaction thermodynamic data	9,400+
Gas phase ion energetics data	14,300+
IR spectrum	7,500+
Mass spectrum	10,600+
UV/Vis spectrum	400+
Vibrational & electronic energy levels	3,300+

Constants of diatomic molecules	600+
Fluid property data	16

February 2000

- Second ion-clustering database added.
- Initial set of 3-d structures added.
- Gas phase heat capacity database added.
- Additional UV/Vis spectra added.
- Updates provided for many of the datasets previously added to the site.
- Database contents (35,900+ Total species):

Data Type	Number of Species
Gas phase thermochemical data	6,100+
Condensed phase thermodynamic data	5,600+
Phase change thermodynamic data	9,500+
Reaction thermodynamic data	9,800+
Gas phase ion energetics data	14,600+
Gas phase ion cluster data	1,300+
IR spectrum	7,500+
Mass spectrum	10,600+
UV/Vis spectrum	400+
Vibrational & electronic energy levels	3,800+
Constants of diatomic molecules	600+
Fluid property data	16

July 2001

- Added limited data from the NIST-TRC source database.
- Added new enthalpy of fusion database.
- Added fluid property models for 17 new fluids.
- Added new capabilities to the fluid models including isochors and some transport properties.
- Updates provided for many of the datasets previously added to the site.
- Database contents (~40,000 Total species):

Data Type	Number of Species
Gas phase thermochemical data	6,500+
Condensed phase thermodynamic data	5,600+
Phase change thermodynamic data	13,800+
Reaction thermodynamic data	9,800+
Gas phase ion energetics data	15,600+
Gas phase ion cluster data	1,100+
IR spectrum	8,700+
Mass spectrum	12,600+
UV/Vis spectrum	400+

Vibrational & electronic energy levels	4,100+
Constants of diatomic molecules	600+
Fluid property data	33

March 2003

- Added group additivity based tool for estimation of gas phase thermochemical properties.
- Added reaction search option.
- Added a large collection of IR spectra.
- Added over 800 UV/Vis spectra.
- Updates provided for many of the datasets previously added to the site.
- Database contents (~48,000 Total species):

Data Type	Number of Species
Gas phase thermochemical data	6,700+
Condensed phase thermodynamic data	6,600+
Phase change thermodynamic data	13,800+
Reaction thermodynamic data	9,800+
Gas phase ion energetics data	15,600+
Gas phase ion cluster data	1,100+
IR spectrum	16,000+
Mass spectrum	15,000+
UV/Vis spectrum	1,600+
Vibrational & electronic energy levels	4,400+
Constants of diatomic molecules	600+
Fluid property data	34

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